Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.16e-11 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 2.51e-01

Confidence level: 7.91e-01

Nearest Neighbors from the Training Set

Image not found
(E)-Crotonaldehyde
Measured: 3.61e-11
Predicted: 3.73e-11

Image not found
Crotonaldehyde
Measured: 3.61e-11
Predicted: 3.73e-11

Image not found
(2E)-3-Phenylprop-2-enal
Measured: 4.80e-11
Predicted: 5.31e-11

Image not found
(Z)-1,2-Dichloroethylene
Measured: 2.48e-12
Predicted: 2.80e-12

Image not found
(E)-1,2-Dichloroethylene
Measured: 2.48e-12
Predicted: 2.80e-12

Image not found
(2E)-2-Hexenal
Measured: 4.40e-11
Predicted: 4.31e-11

Image not found
Glutaraldehyde
Measured: 2.38e-11
Predicted: 2.50e-11